Spin-phonon relaxation from a universal ab-initio density-matrix approach

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Abstract
Designing new quantum materials with long-lived electron spin states urgently requires a general theoretical formalism and computational technique to reliably predict intrinsic spin relaxation times. We present a new, accurate and universal first-principles methodology based on Lindbladian dynamics of density matrices to calculate spin-phonon relaxation time of solids with arbitrary spin mixing and crystal symmetry [1]. This method describes contributions of Elliott-Yafet (EY) and D'yakonov-Perel' (DP) mechanisms to spin relaxation for systems with and without inversion symmetry on an equal footing. We show that intrinsic spin and momentum relaxation times both decrease with increasing temperature; however, for the DP mechanism, spin relaxation time varies inversely with extrinsic scattering time. We predict large anisotropy of spin lifetime in transition metal dichalcogenides. The excellent agreement with experiments for a broad range of materials underscores the predictive capability of our method for properties critical to quantum information science [2-5].

REFERENCES

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FIGURES

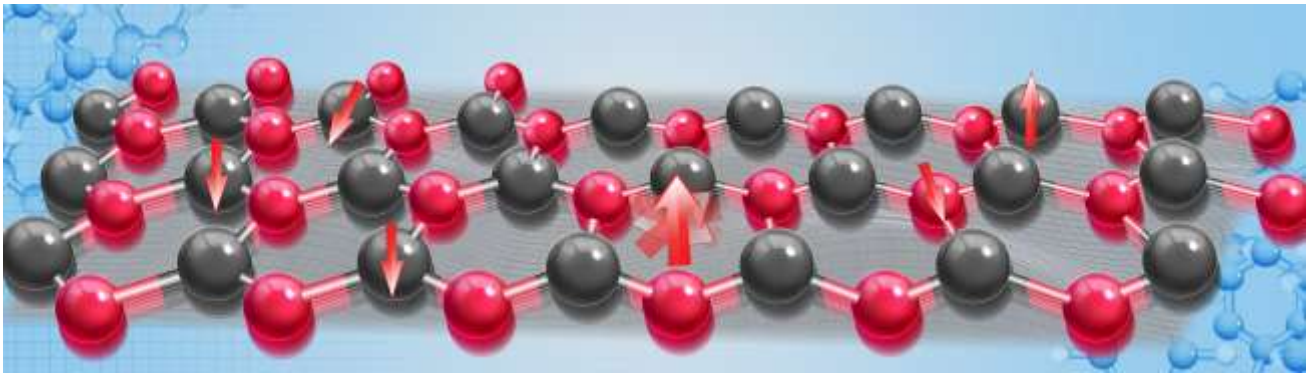

Figure 1: Spin-phonon relaxation in two-dimensional materials